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Title: Casting Modeling of Uranium and Uranium Alloys

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Casting Modeling of Uranium and Uranium Alloys

Deniece R. Korzekwa and Robert M. Aikin, Jr.

The Accelerated Implementation of Materials and Processes: Manufacturing and Processing
November 12, 2003

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Overview

Casting Simulation Goals

Vacuum Induction Melting at LANL

Experimental Set-up

Simulation Set-up

Code comparison

Where now?

Summary and Future Directions

Casting Simulations Goals

- Combined experimental and simulation program
- Perform many computer "experiments" and few actual experiments
- Investigate the feasibility of replacing wrought products with cast components
- Produce castings with a higher metal yield to reduce worker exposure and minimize hazardous and radioactive wastes
- Enable rapid development of optimized weapons alloy casting processes
- Predict and control microstructural features
- Improve constitutive models for performance codes
- Address fine-scale microstructural effects of solidification and melt convection with high resolution simulations and improved physical models

What can we expect from a computer model?

Ideally, we could model all the physics every time with the utmost accuracy

In reality we are often limited by:

- time available
- computer speed and capacity
- mesh resolution and generation
- material property data (especially temperature dependency)
- understanding of boundary conditions and their properties
- inadequate models to describe the underlying physics

and must simplify the problem

> Understanding the current process is the first step to successful implementation of agile manufacturing

We often must decide what are the important features of the process and model these to the best accuracy we can.

Vacuum Induction Melting at LANL

Vacuum – heat transfer by conduction and radiation only
heat transfer across gaps will be by radiation only

Induction heating – electromagnetics important to initial temperature distribution
single coil furnaces – crucible and mold heated with same coil
temperature gradient within the mold

Graphite molds – high conductivity, will act as a heat source or heat sink
must calculate the heat transfer in both the metal and the mold

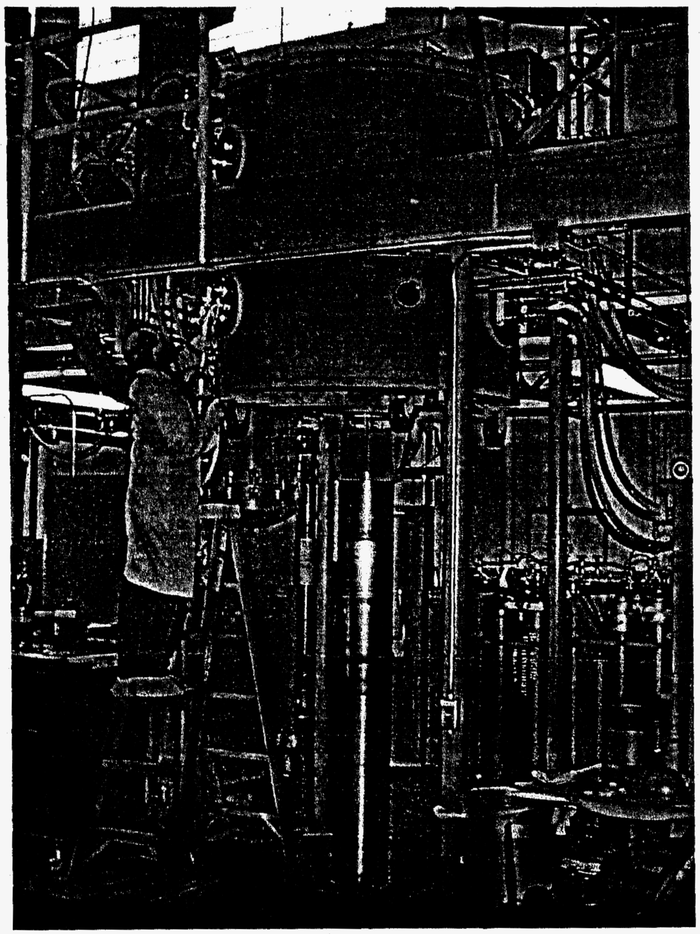
Ceramic mold coating – too thin to model explicitly, barrier to heat transfer

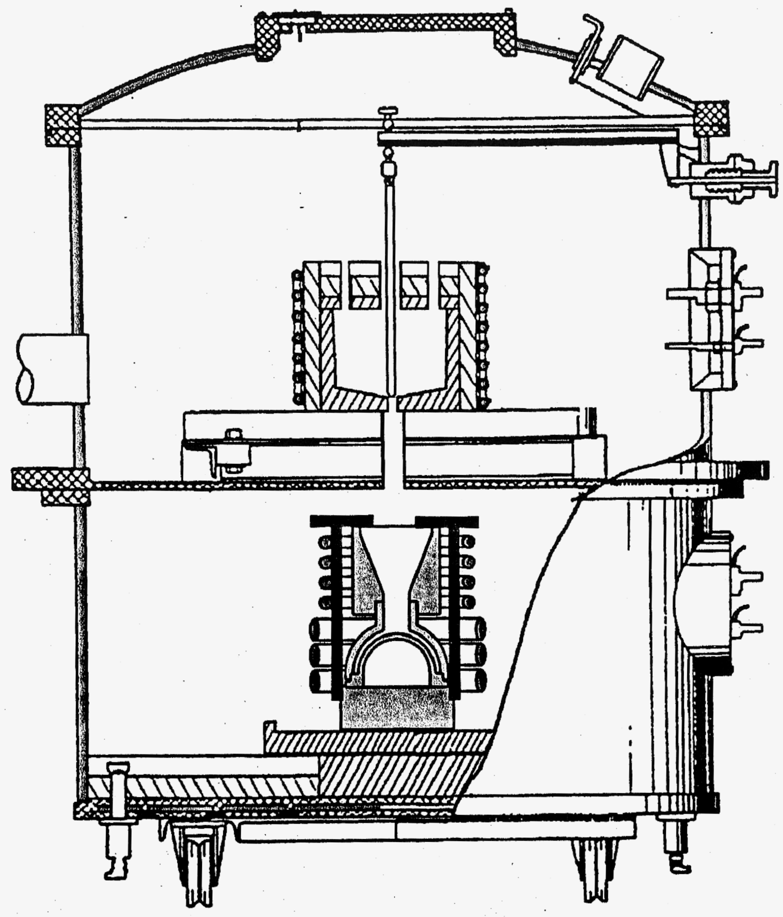
Shrinkage or expansion -- of the metal as it solidifies and cools requires a
Time/stress/position dependent heat transfer coefficient

Alloys – many have a high partition coefficient and species segregation is a problem
at both a macro and micro level

Radioactive materials – many materials properties are unknown, especially high
temperature and temperature dependent properties

Three-Zone Vacuum Induction Furnace (K-Furnace)





Three induction coils:

- **Melting coil (35 kW at 9.6 kHz)**
- **Two mold heating coils (50 kW at 3 kHz)**

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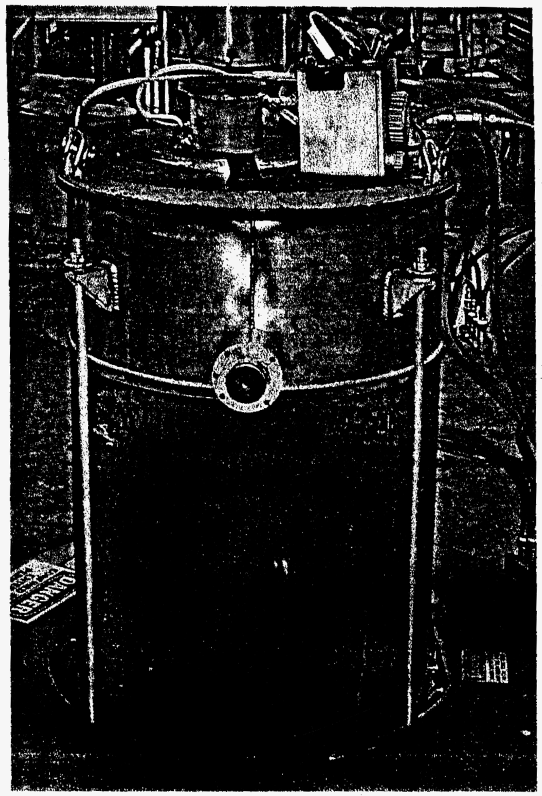
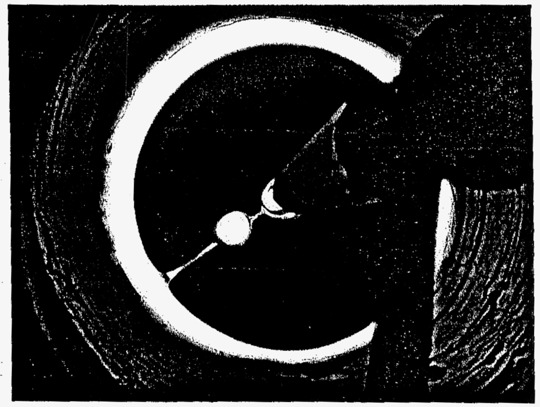
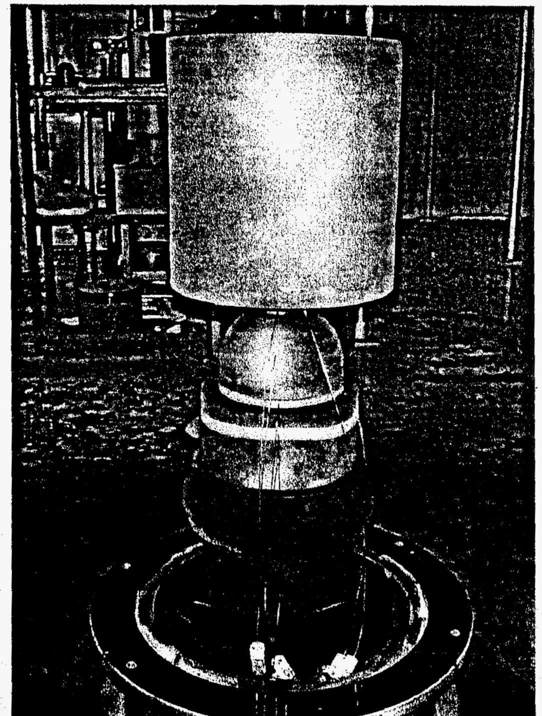
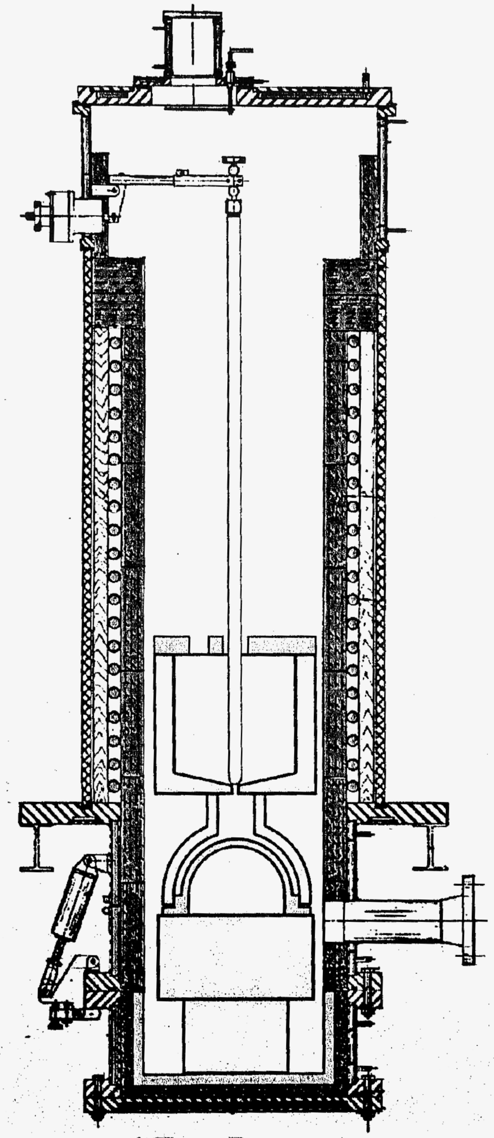
Single-Zone Vacuum Induction Furnace (C-Furnace)









Single induction coil:
- **36" x 18" ϕ**
- **100 kW at 3 kHz**

Thermocouple Layout for DU Hemi 03K-409

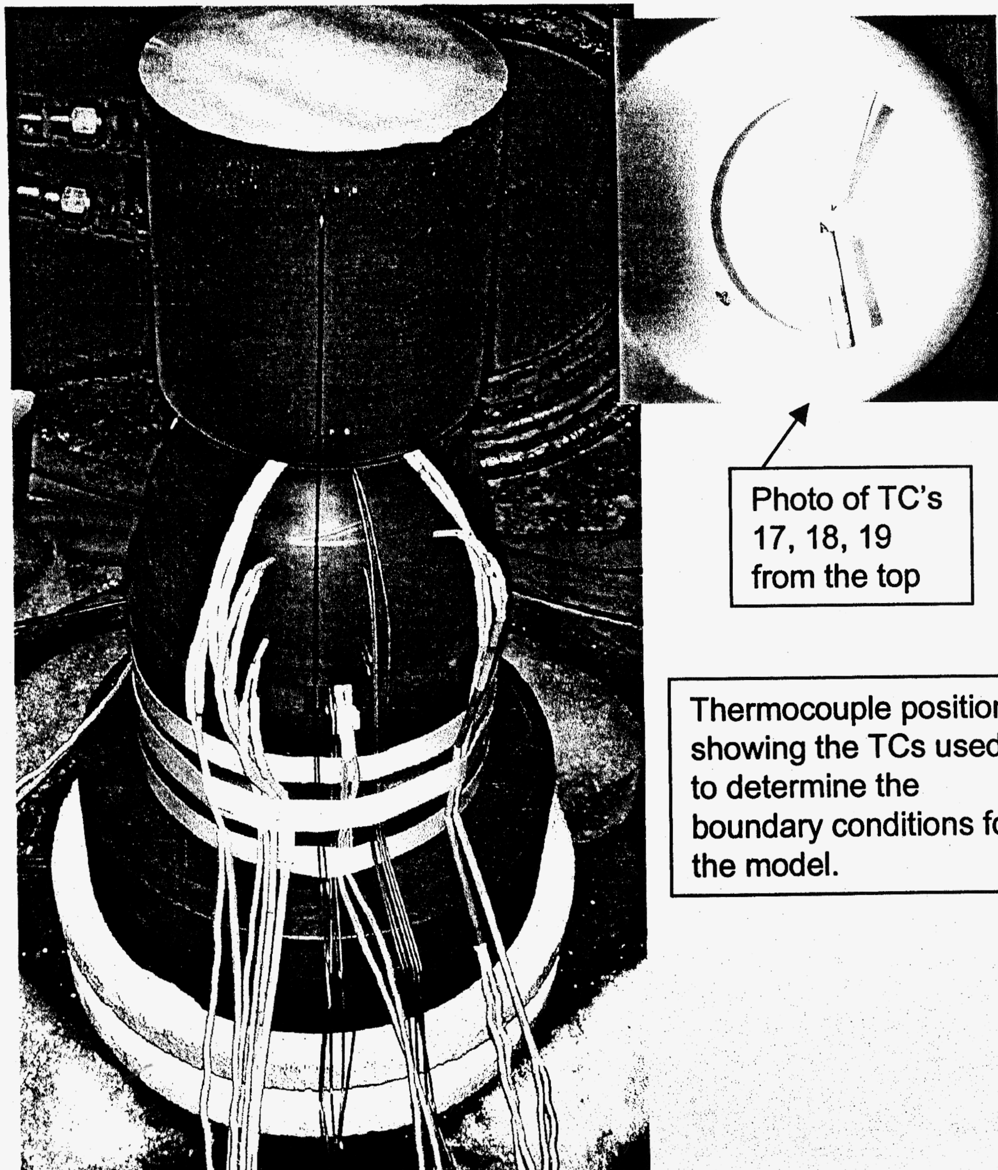
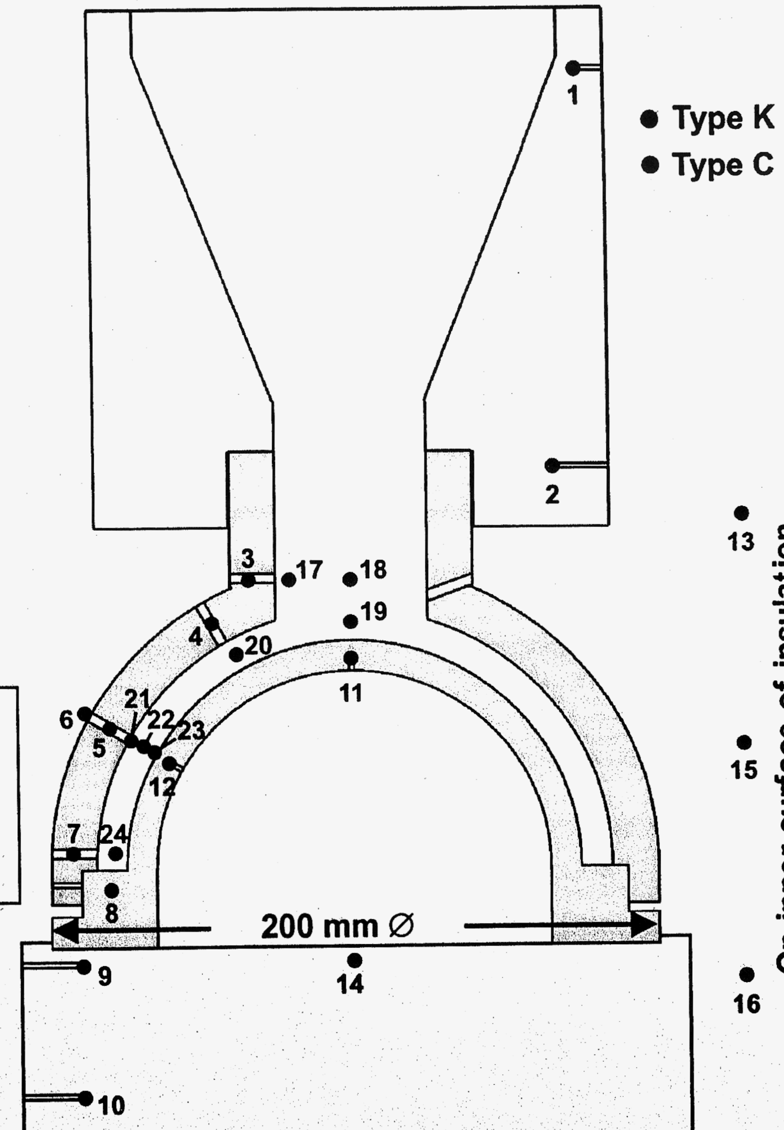
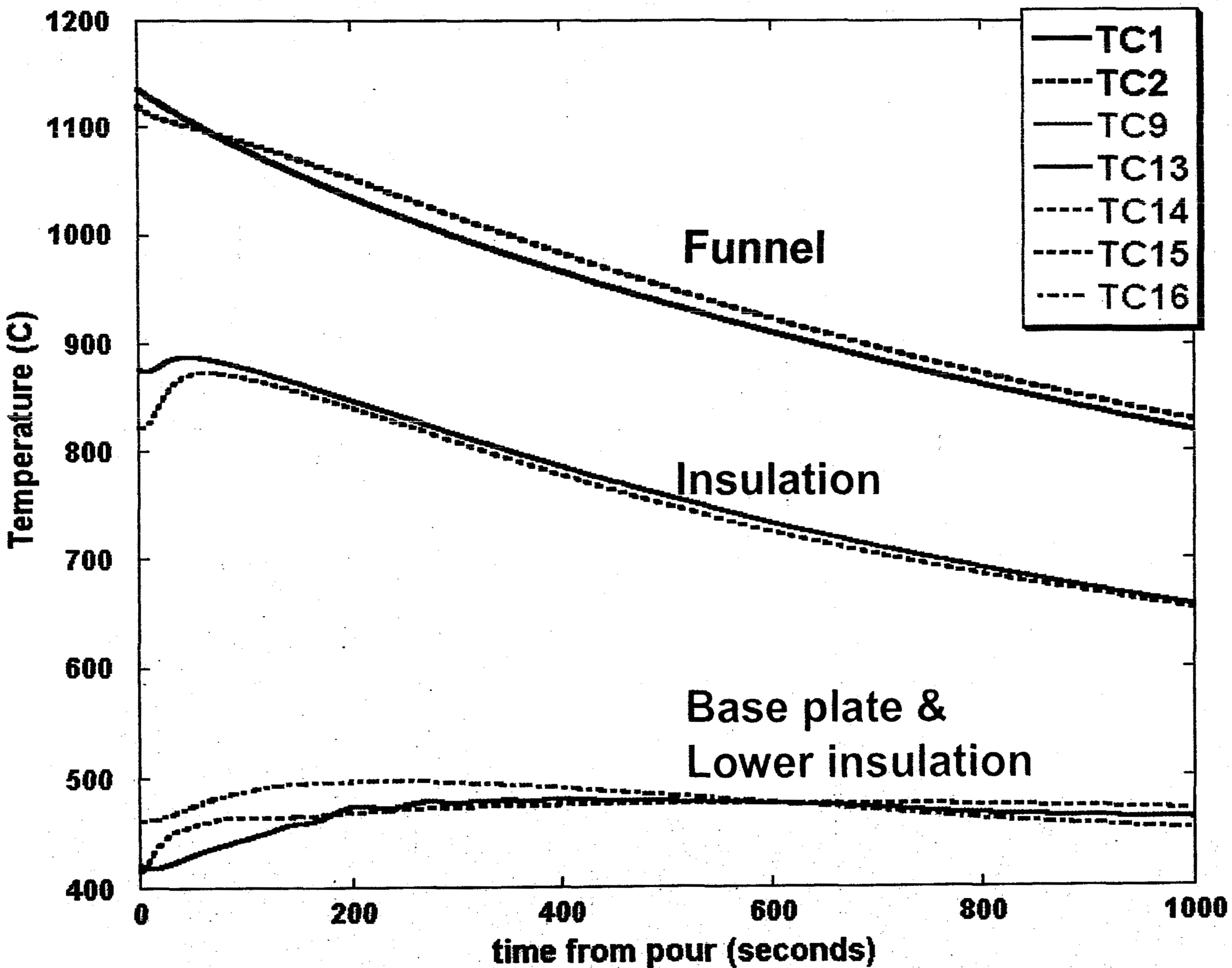


Photo of TC's 17, 18, 19 from the top

Thermocouple positions showing the TCs used to determine the boundary conditions for the model.



Thermocouples used for Boundary Conditions



Simulation Codes Used for this Study

Flow3D

- commercial code
- coupled fluid flow and heat transfer
- simple radiation model
- built-in meshing
- single or multi processor (Open MP)

Truchas

- currently under development at LANL
- filling and fluid flow; heat transfer
- simple radiation model plus view factor model
- no mesh generation, must use other software
- electro-magnetics model (not used for this comparison)
- multi-processors (MPI)

ProCAST

- commercial code
- couple fluid flow and heat transfer
- view factor radiation model
- meshcast meshing code
- electro-magnetics model (not used for this comparison)
- single processor (multi-processing being tested)

Simulation Setup – All Codes

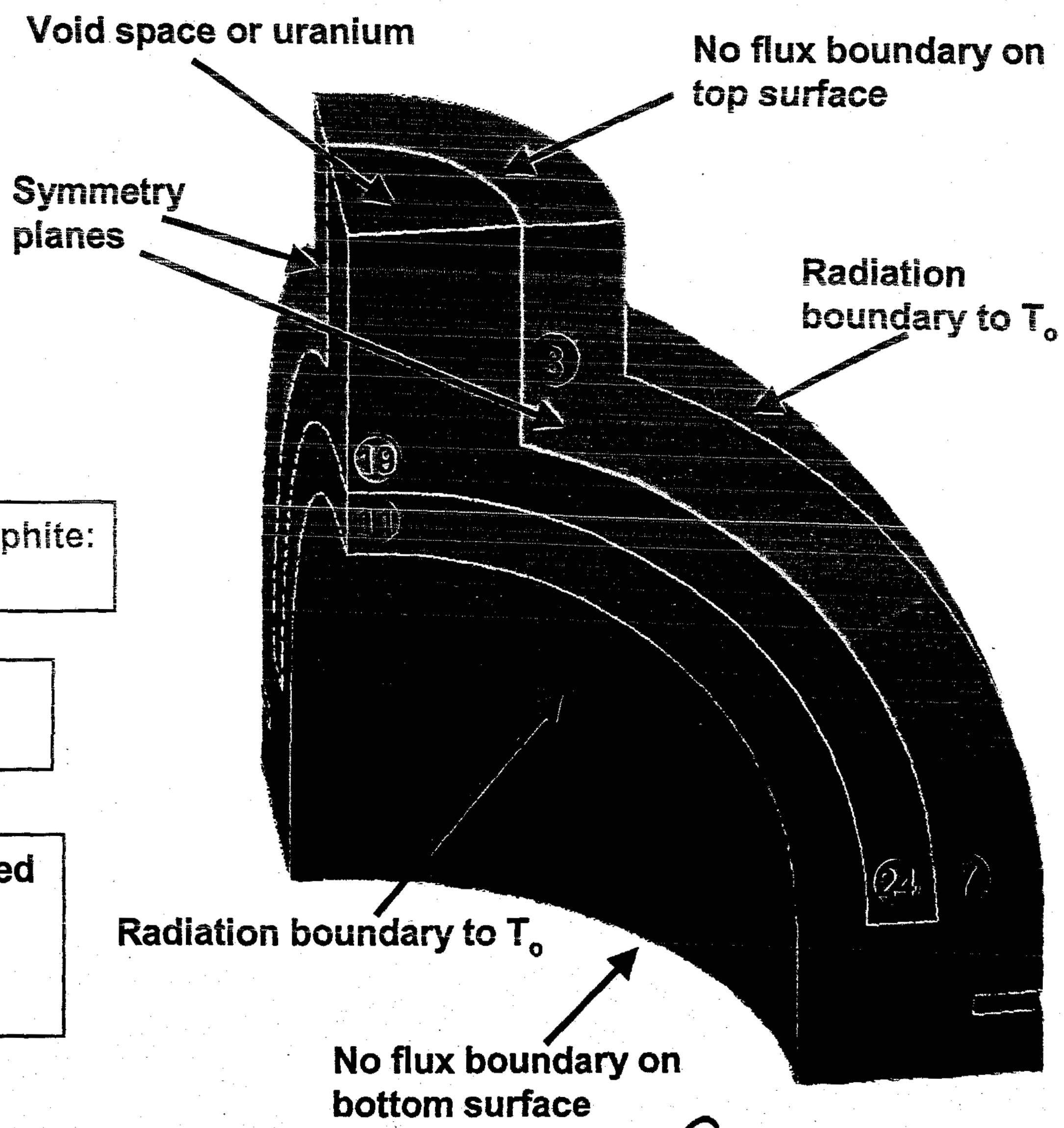
Initial mold temperature varies to match starting conditions:
Red – 1300C
Purple – 700C
(from experimental data)
No electromagnetics used.

Uranium - 1300C (both filling and non-filling)

Heat transfer coefficient: metal and graphite: htc= 2000 W/m²K

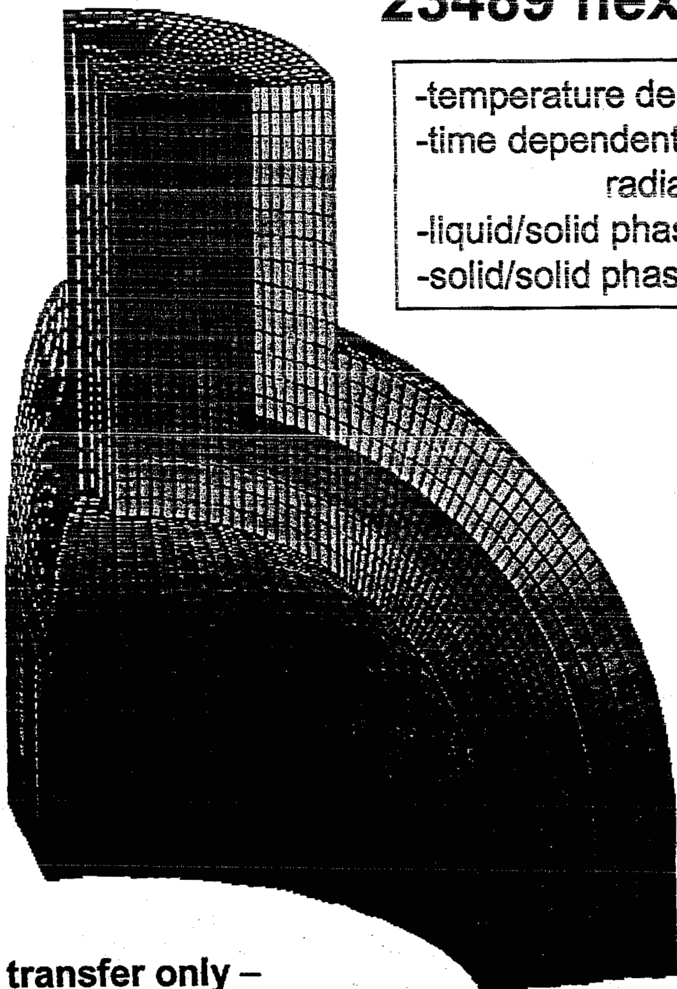
Radiation boundary condition: $\epsilon = 0.4$
T_o Varies depending on code

Position and type of thermocouples used for comparison are shown:
red – type K in the graphite
blue – type C in the metal

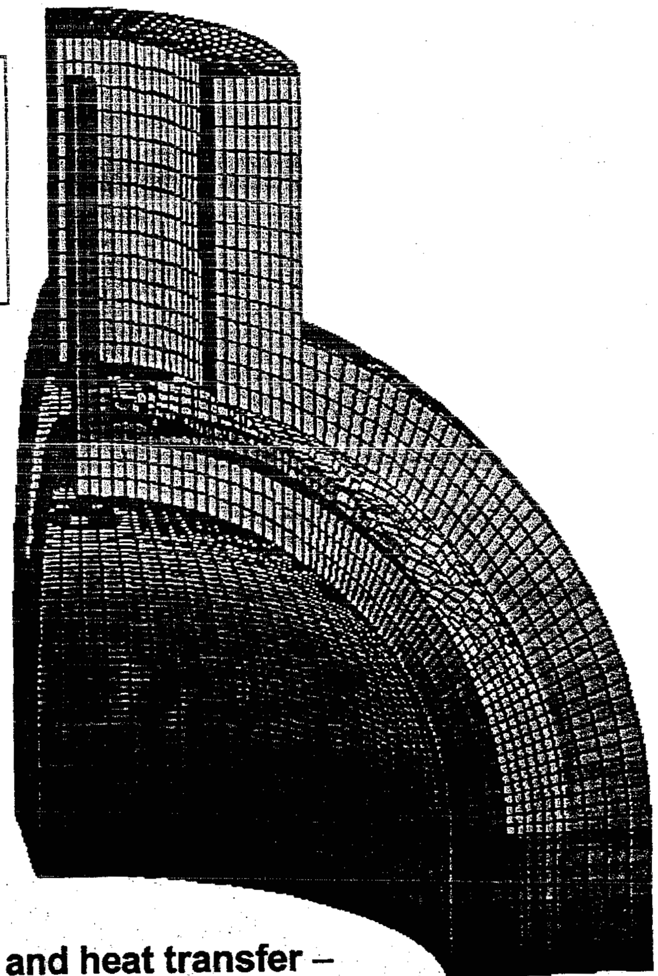


Simulation Setup - Truchas

23489 hex elements



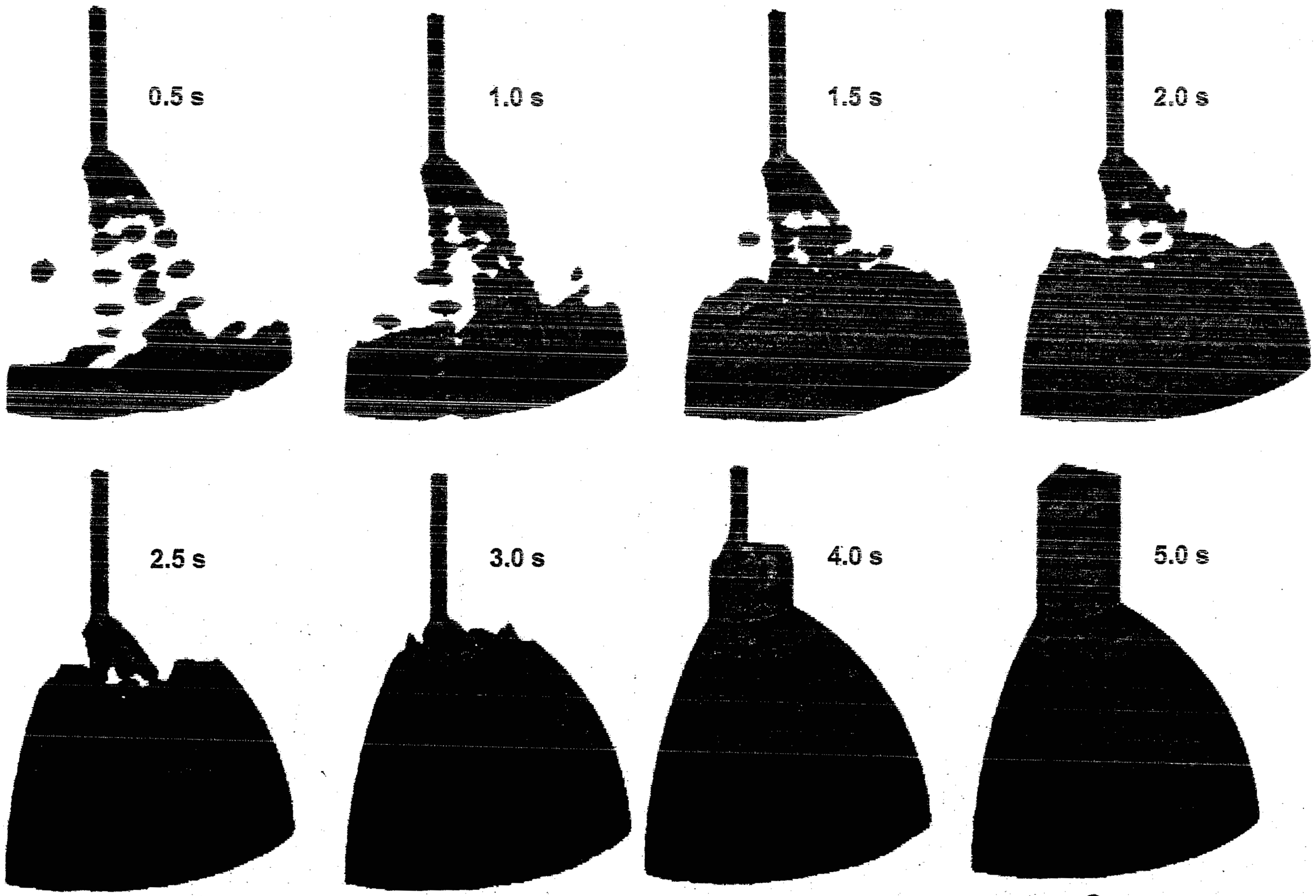
- -temperature dependent properties
- -time dependent /position dependent radiation boundary
- -liquid/solid phase change
- -solid/solid phase change



Heat transfer only –
4 processors ES45 – 10.0 hours for 1000 seconds simulation time

Filling and heat transfer –
4 processors ES45 – 34.0 hours for 5 seconds simulation time

Filling – Truchas

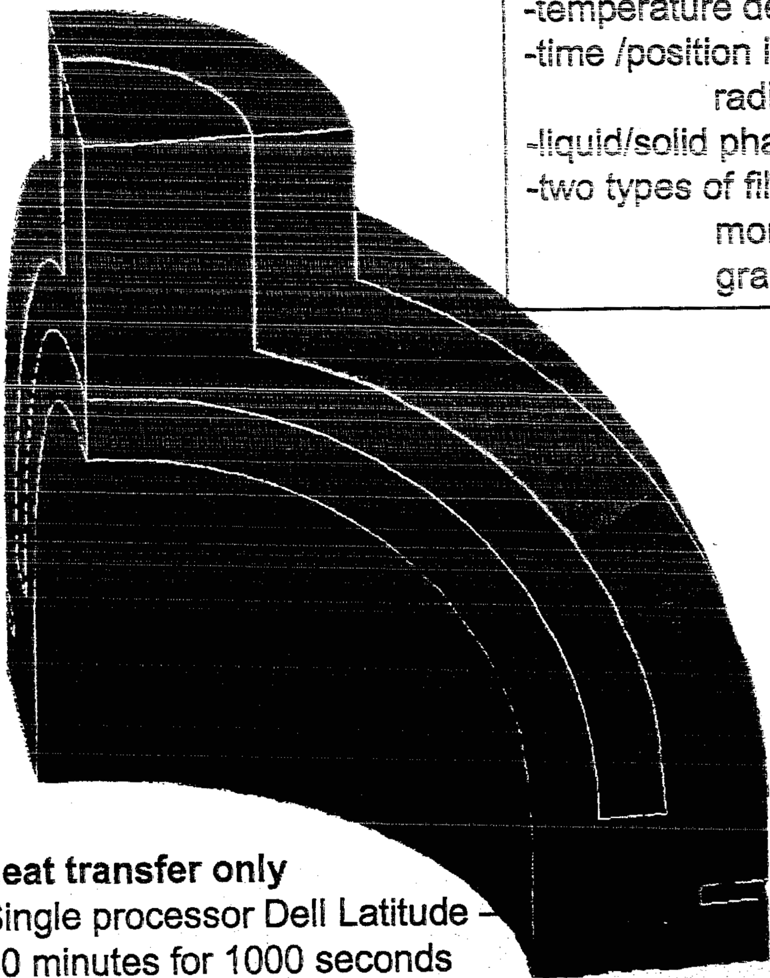


Showing isovolume only

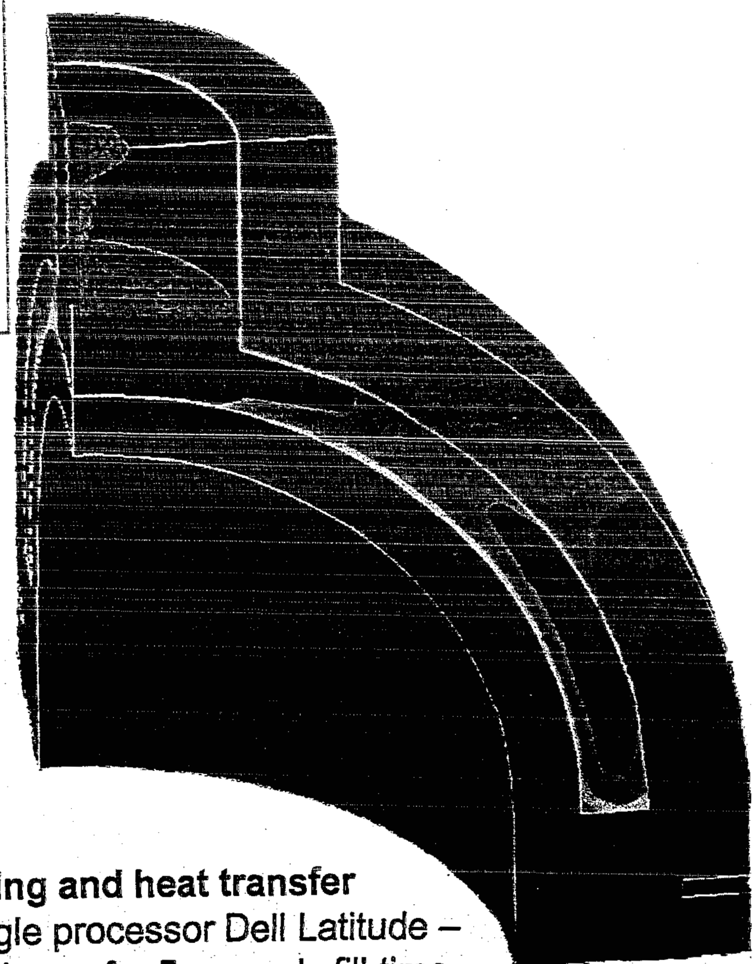
Simulation Setup - ProCAST

198061 tet elements

- -temperature dependent properties
- -time /position independent radiation boundary
- -liquid/solid phase change
- -two types of filling:
  - momentum dominated
  - gravity dominated



heat transfer only
Single processor Dell Latitude –
50 minutes for 1000 seconds simulation time



Filling and heat transfer
Single processor Dell Latitude –
5.3 hours for 5 seconds fill time
2.75 hours for 1000 sec simulation time

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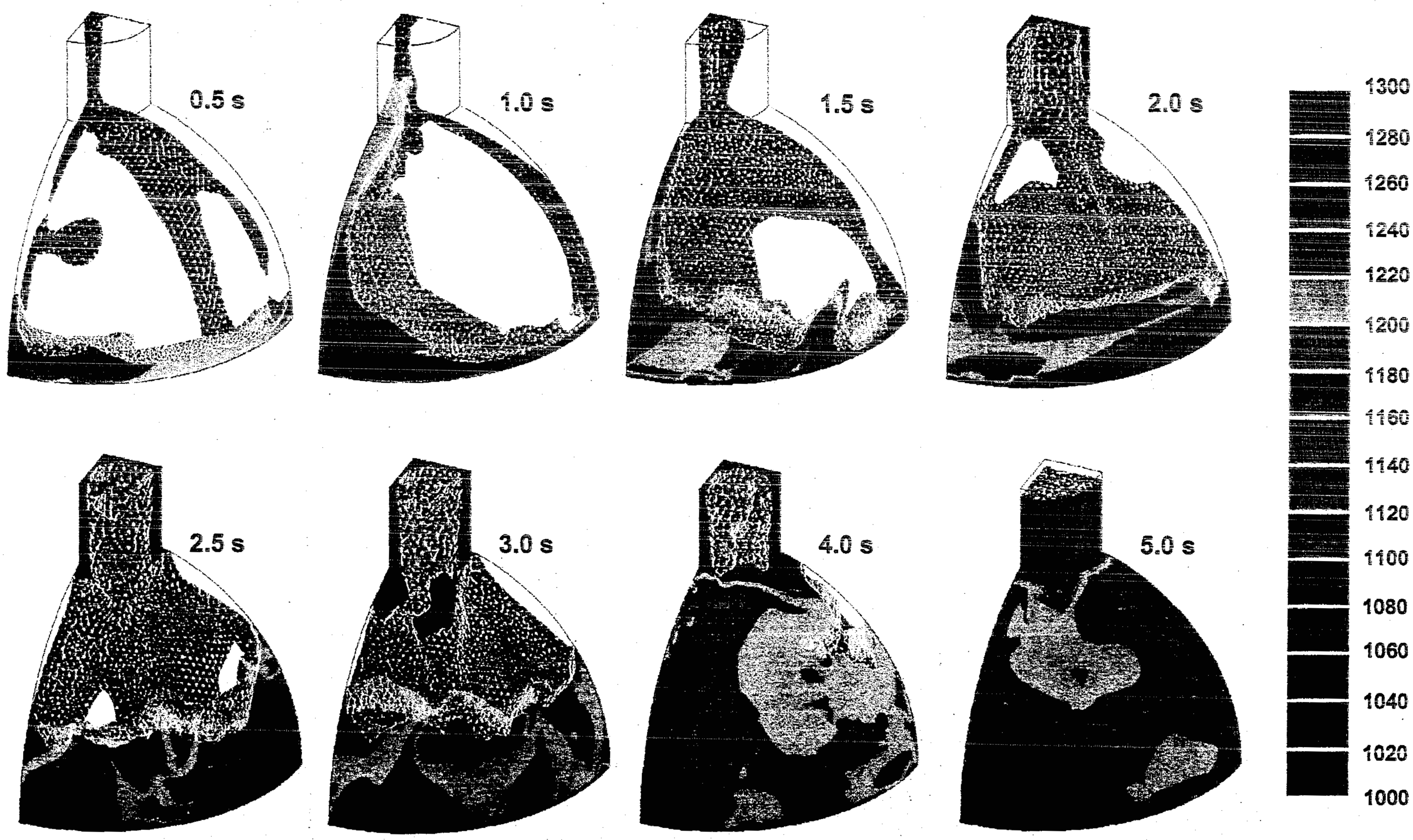
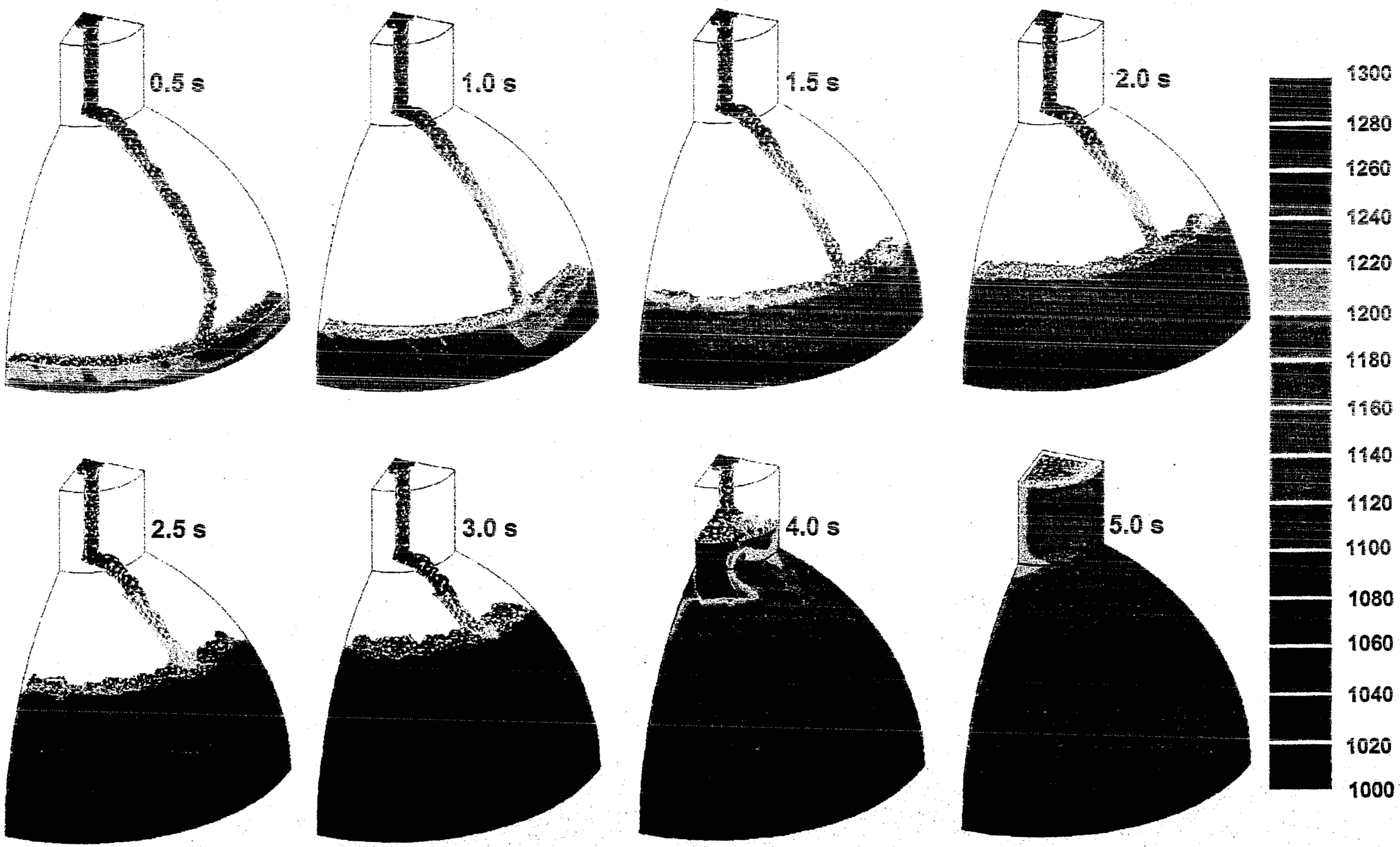
ProCAST – Filling Type 1 –momentum dominated

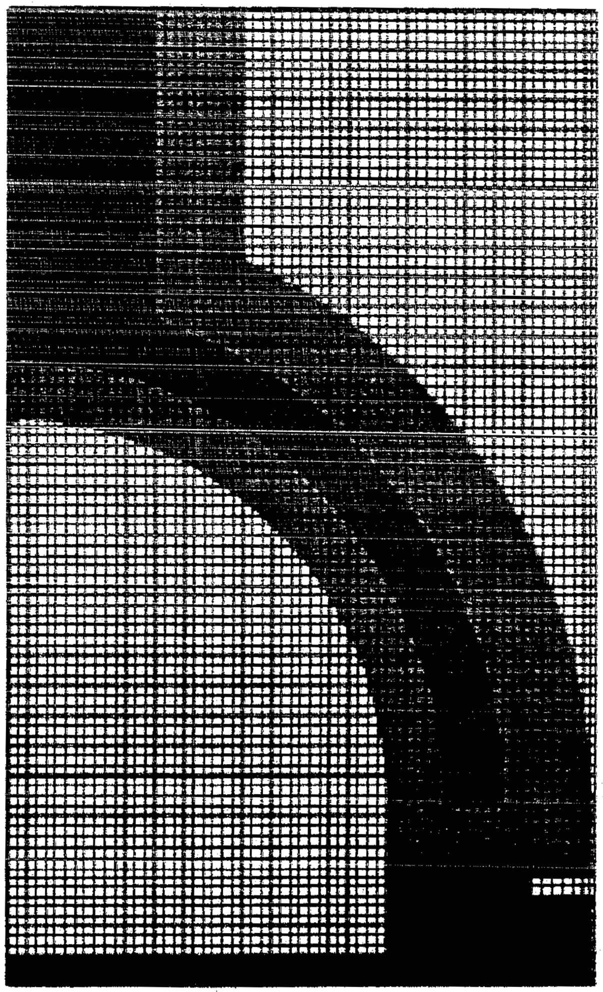


ProCAST - Filling   Type 2 –gravity dominated



Simulation Setup - Flow3D

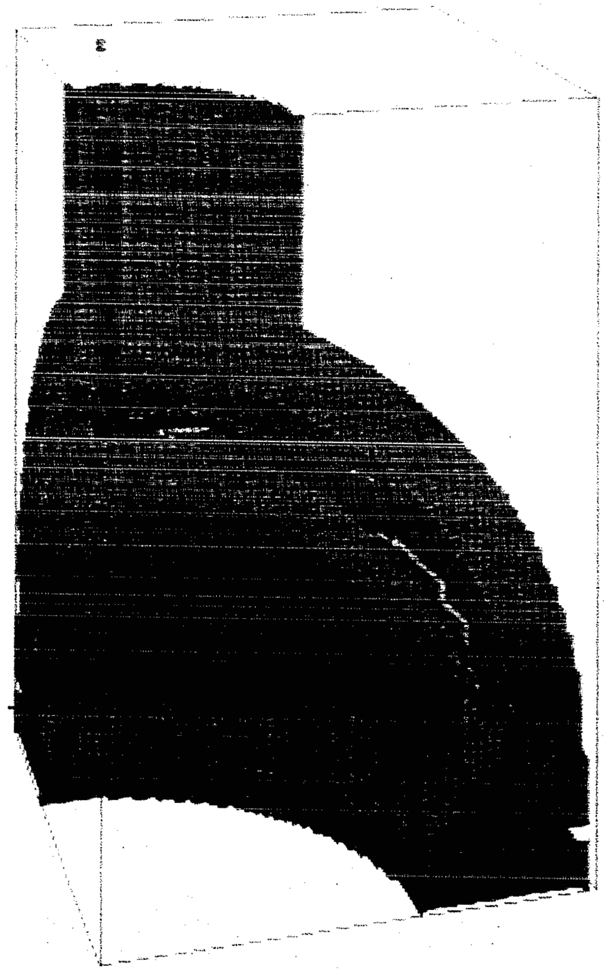
2D Axisymetric - 5978 Cells



No filling, heat transfer and fluid flow
1 processor ES45 - 103 sec for
1000 seconds of simulation time

- temperature independent mold properties
- time dependent top temperature BC / time independent bottom temperature BC
- time independent radiation boundaries
- liquid/solid phase change
- solidification shrinkage

3D - 408807 Cells



Filling and heat transfer
4 processors ES45 - 23.4 hours for
5 seconds of simulation time

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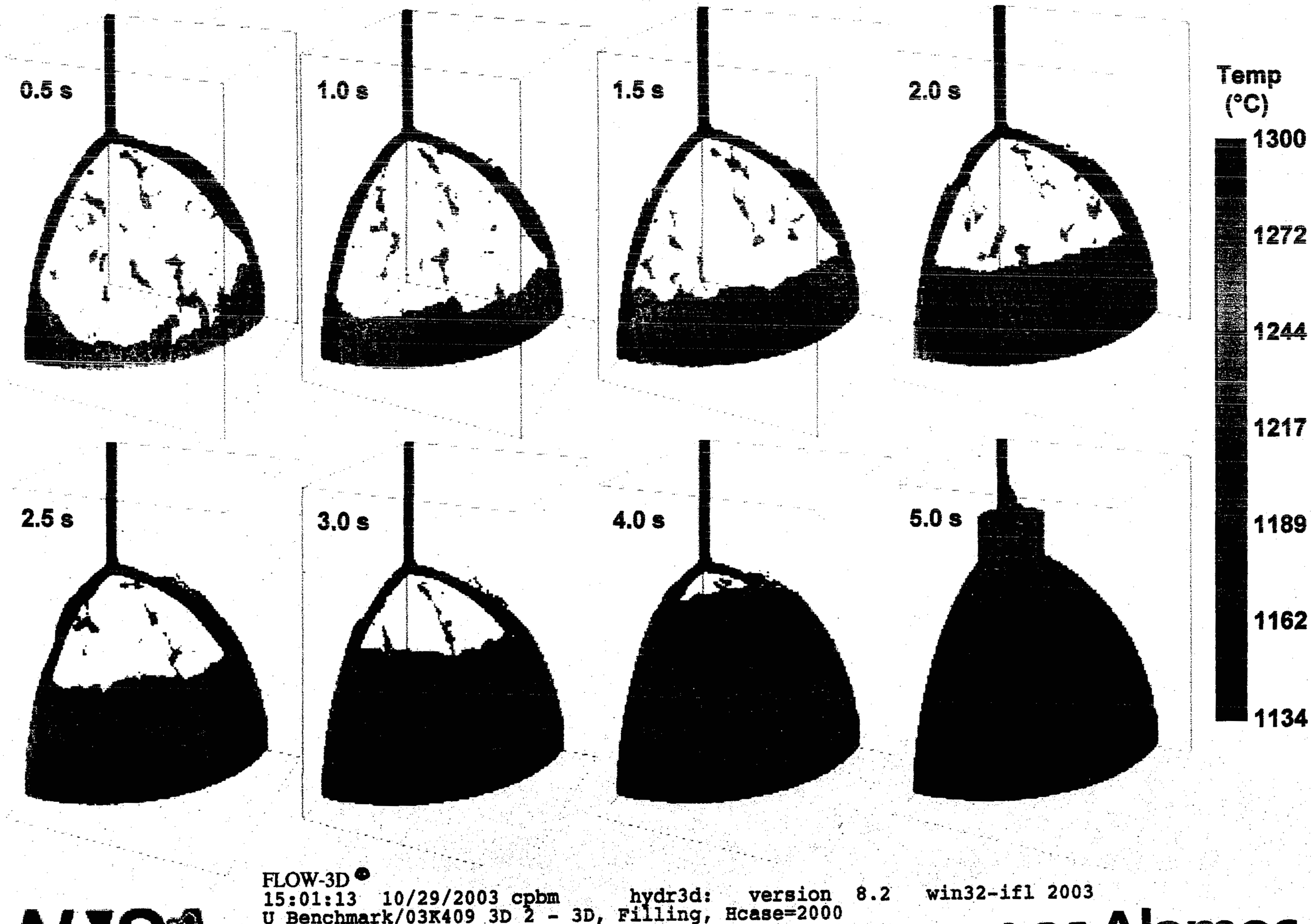
Flow3D - Mold Filling



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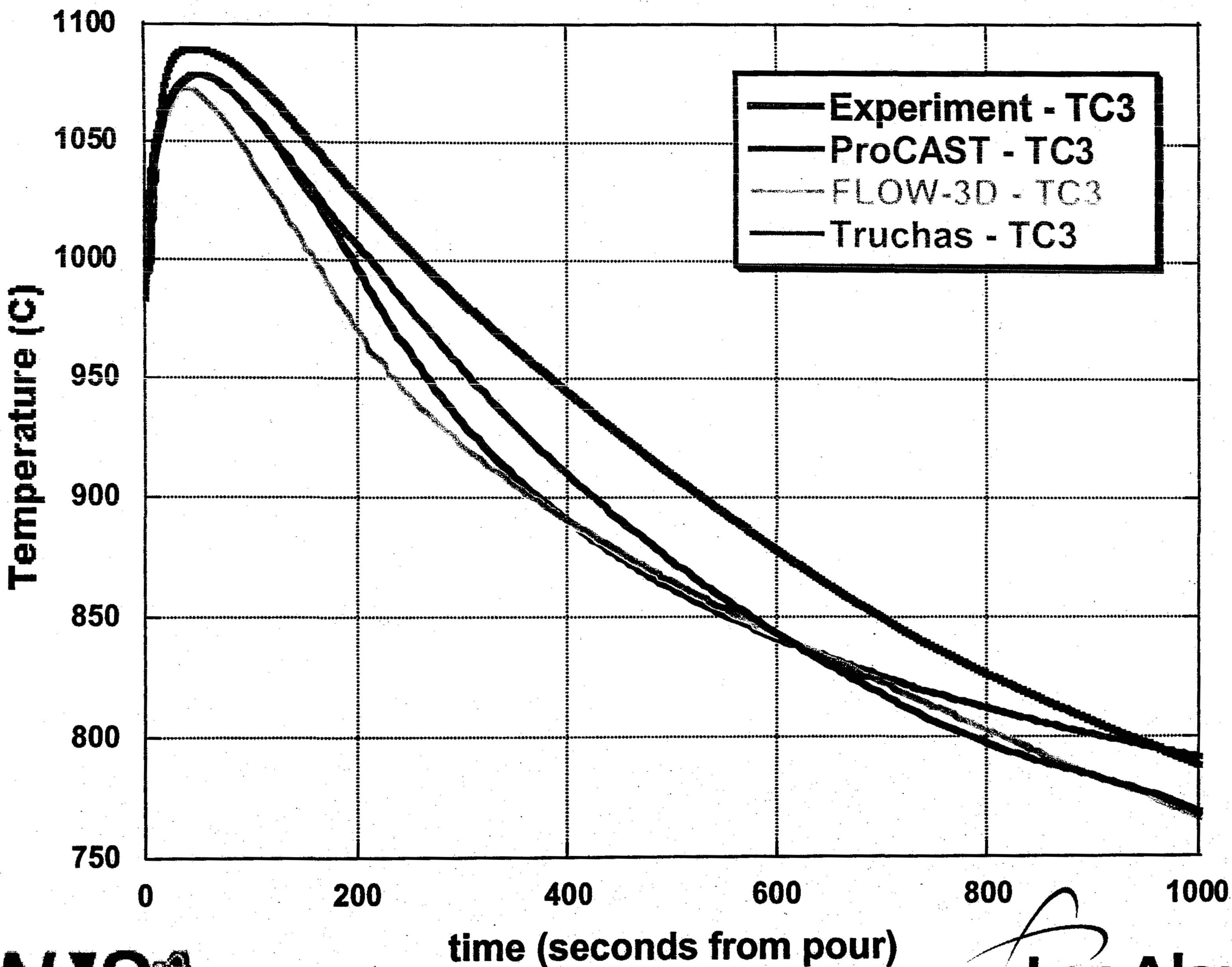
Basic Hemi: 03K-409 Outer Mold Riser



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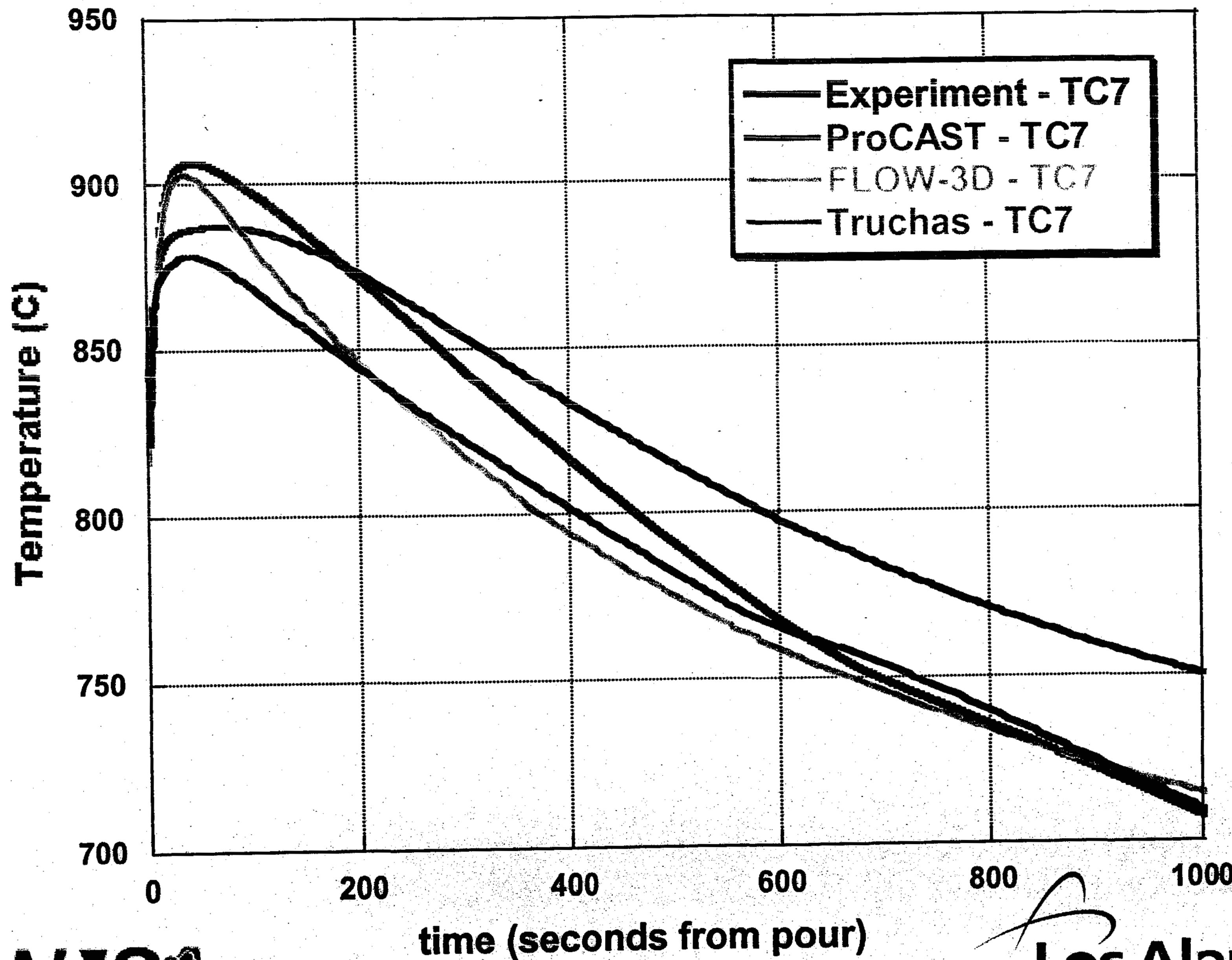
Basic Hemi: 03K-409 Outer Mold Bottom



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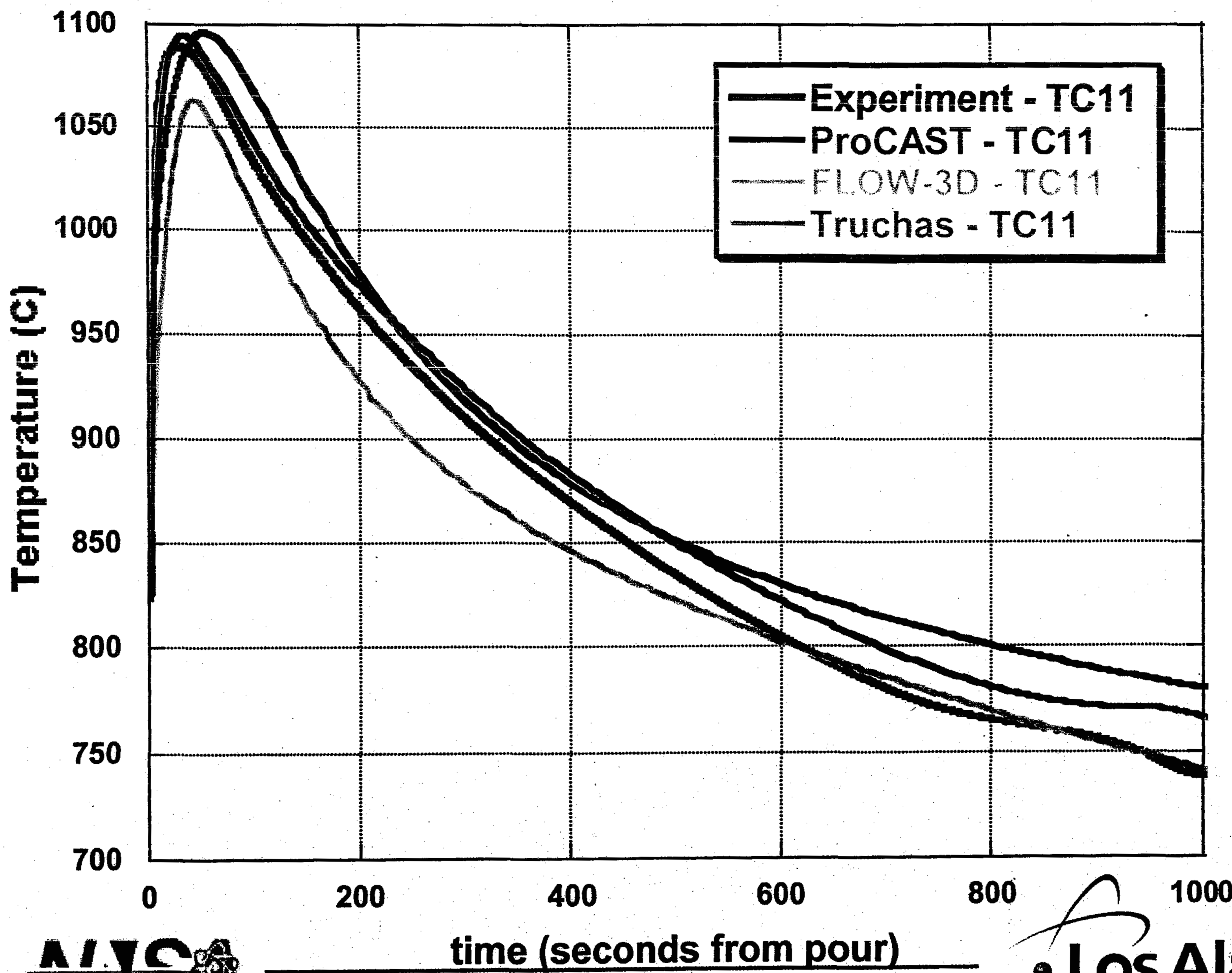
Basic Hemi: 03K-409 Inner Mold Pole



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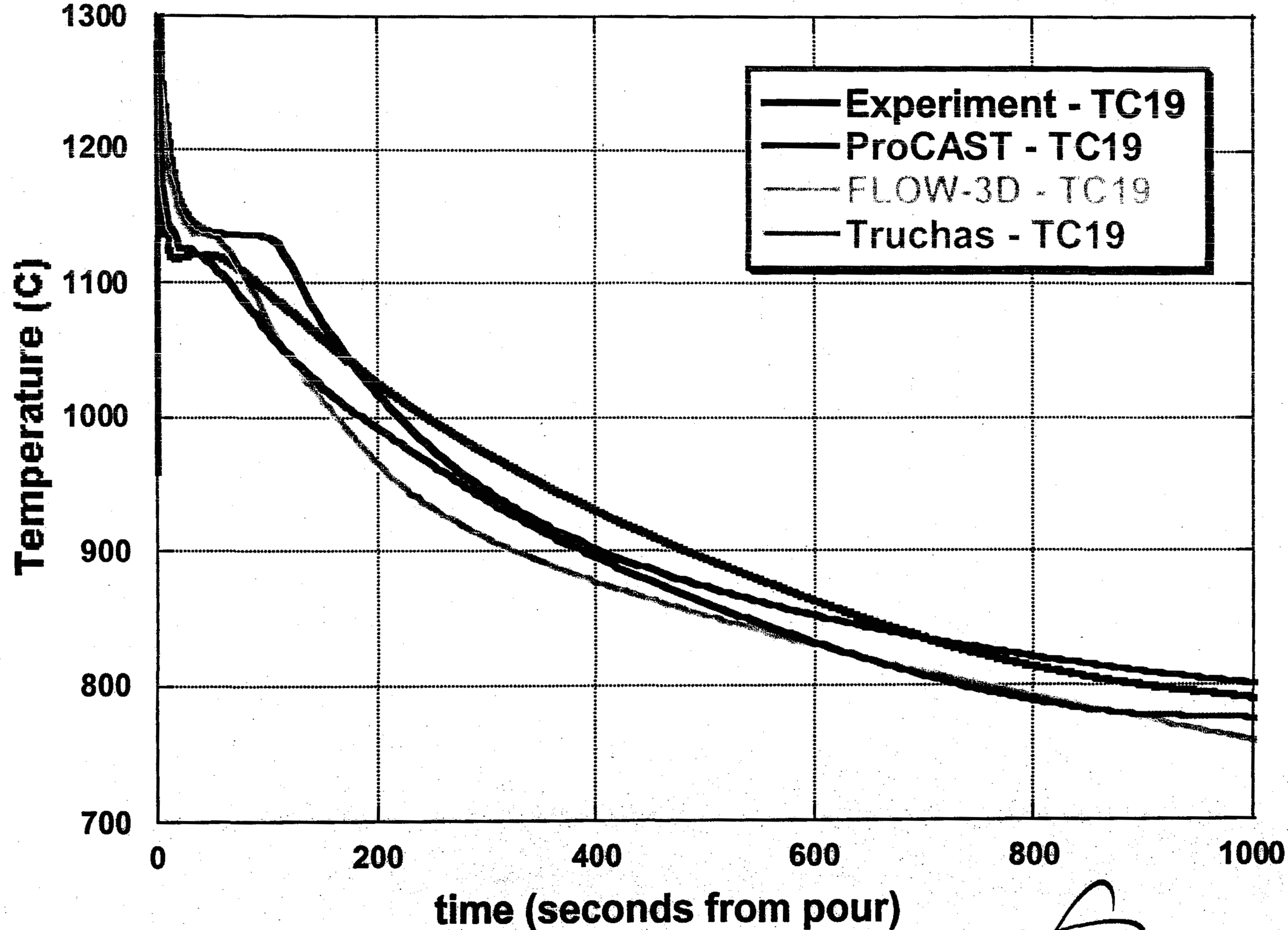
Basic Hemi: 03K-409 Metal Pole



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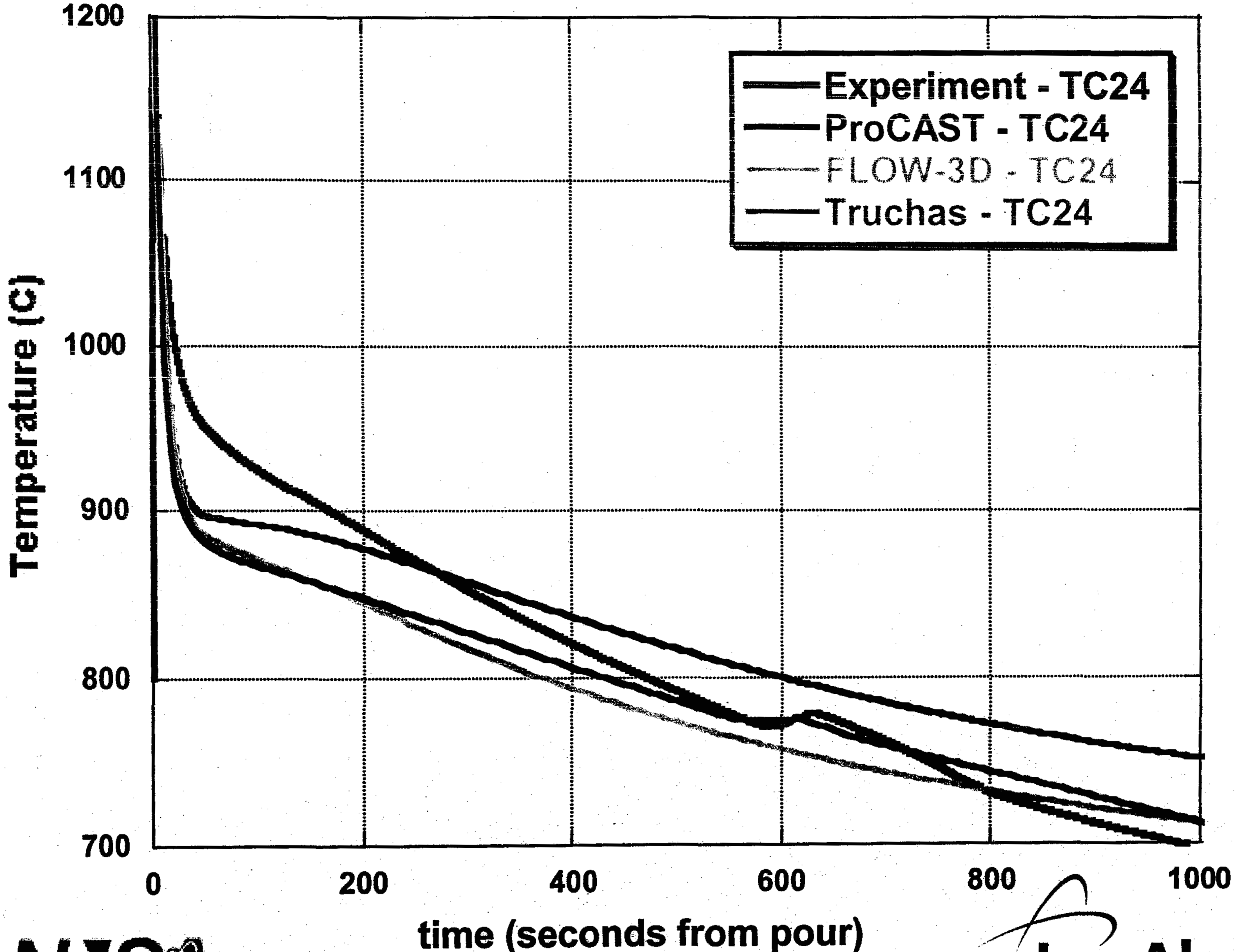
Basic Hemi: 03K-409 Metal Bottom



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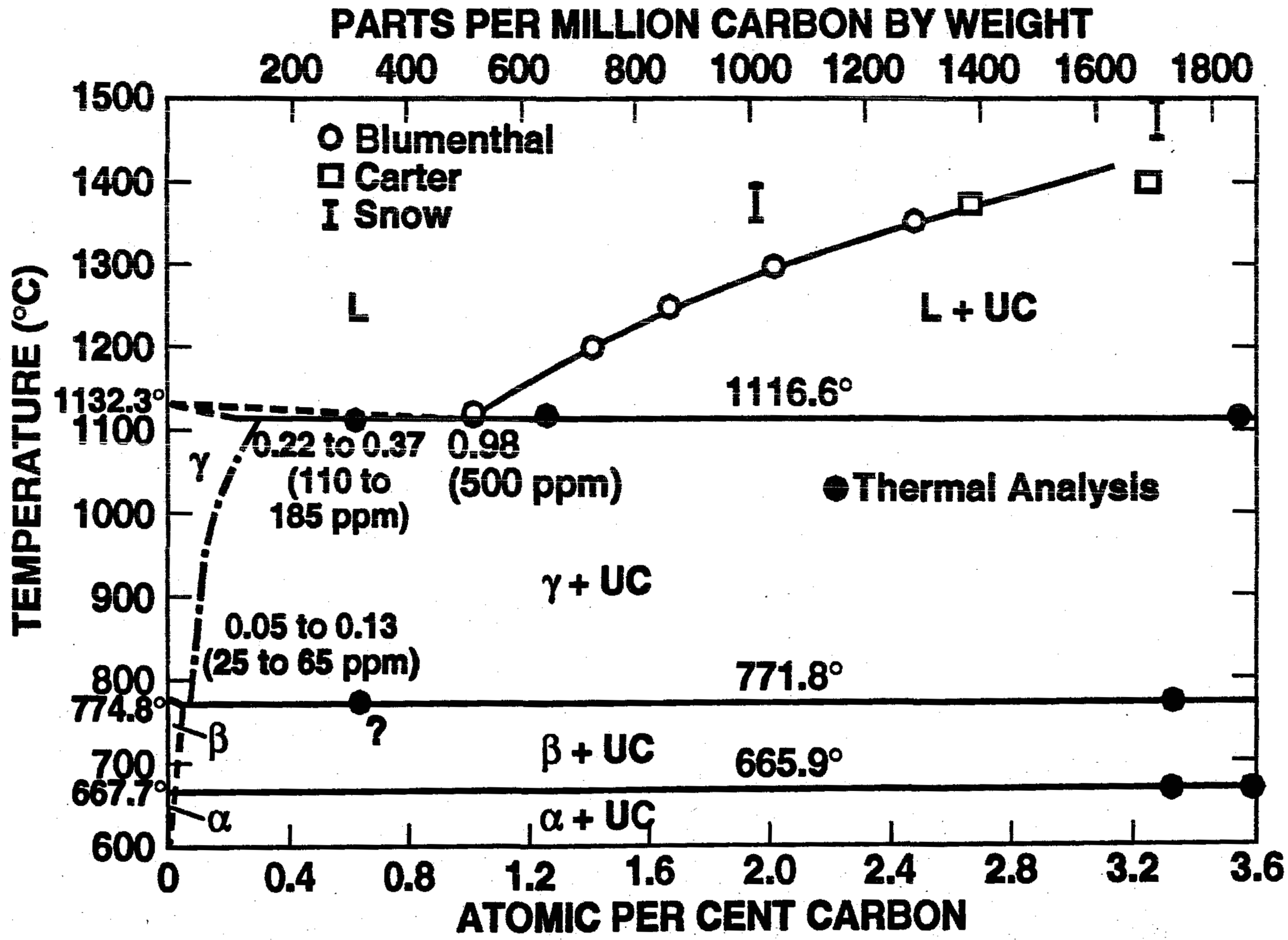
Uranium-Carbon Phase Diagram

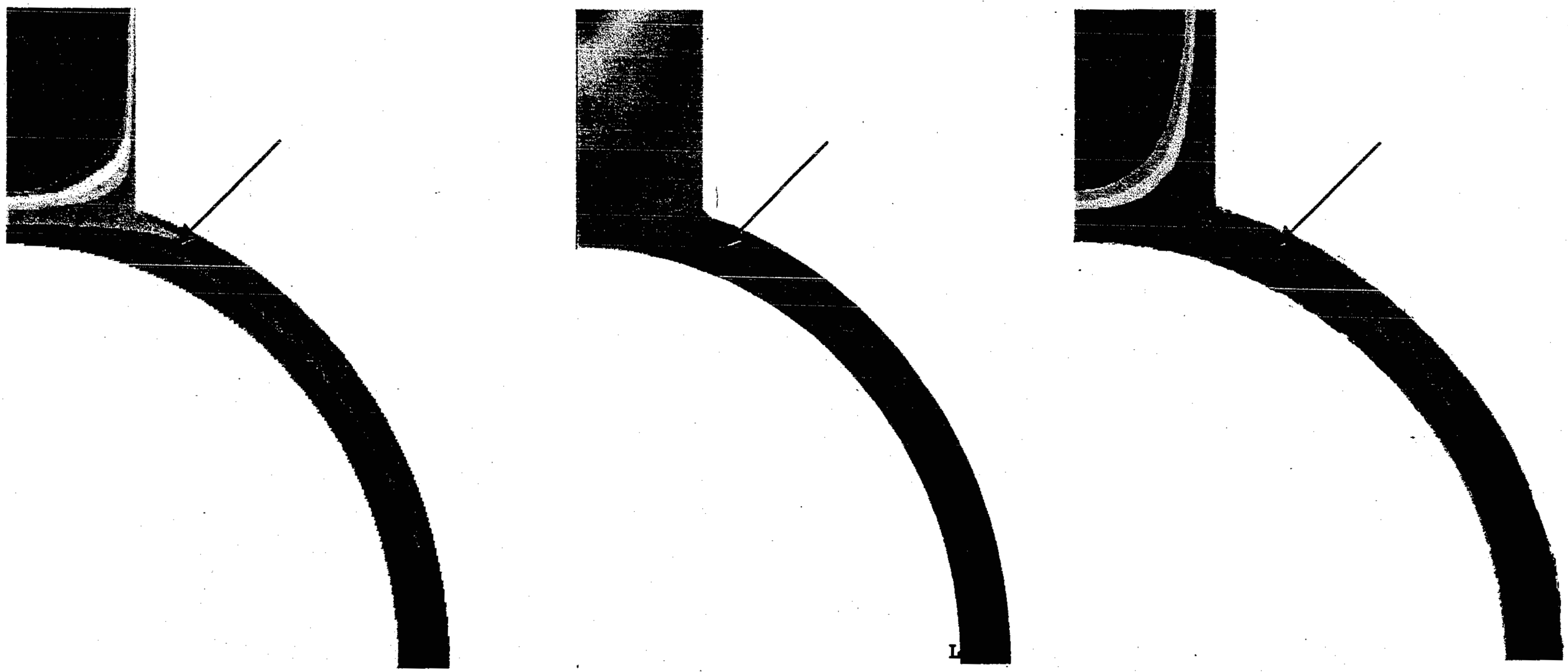


Uranium - Carbon Phase Diagram

B. Blumenthal, *J. of Nuclear Mat.*, 2 #3, p.197 (1960)

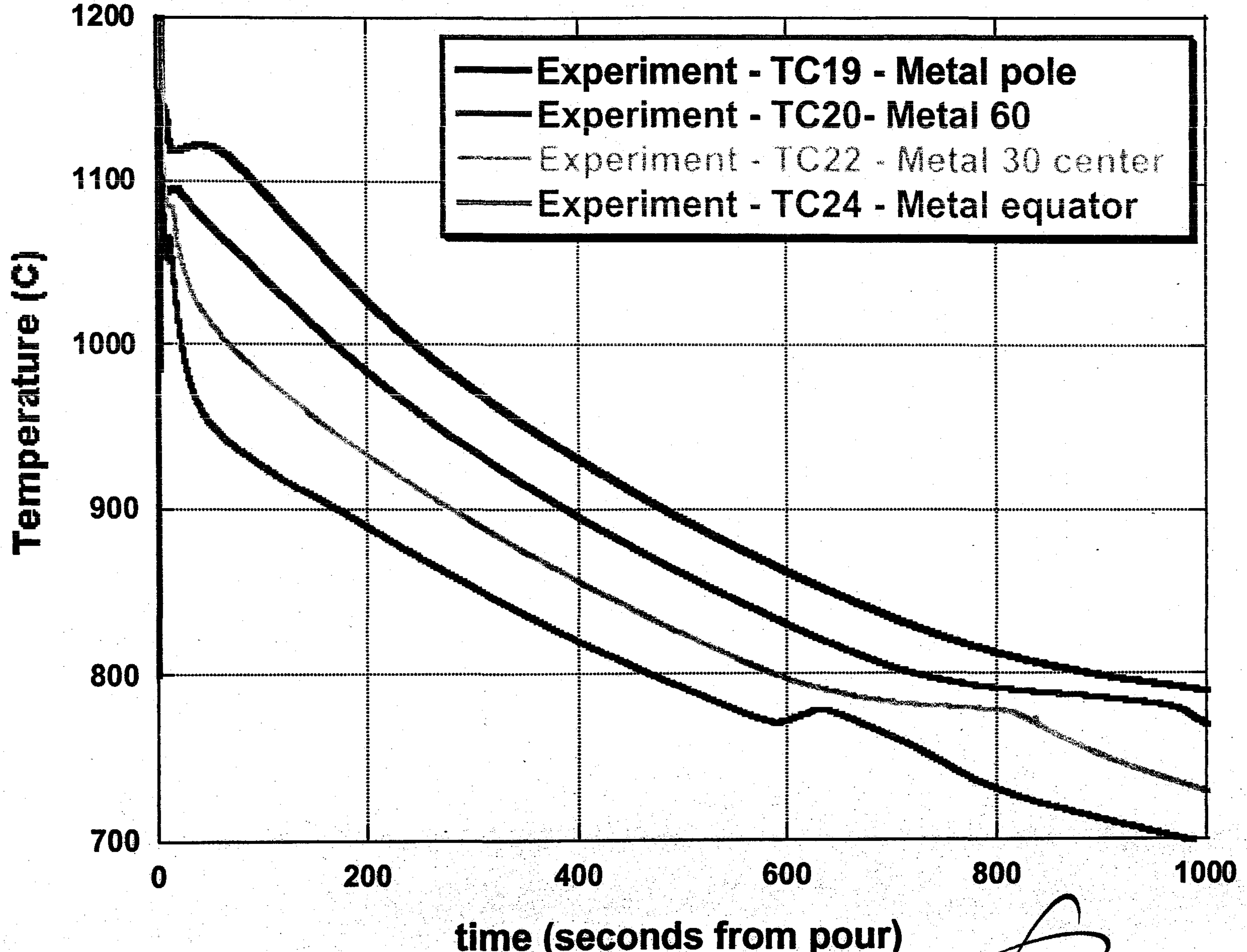
Time to Solidification

Arrows at 25 seconds



Truchas FLOW-3D ProCAST

Basic Hemi: Metal Temperatures



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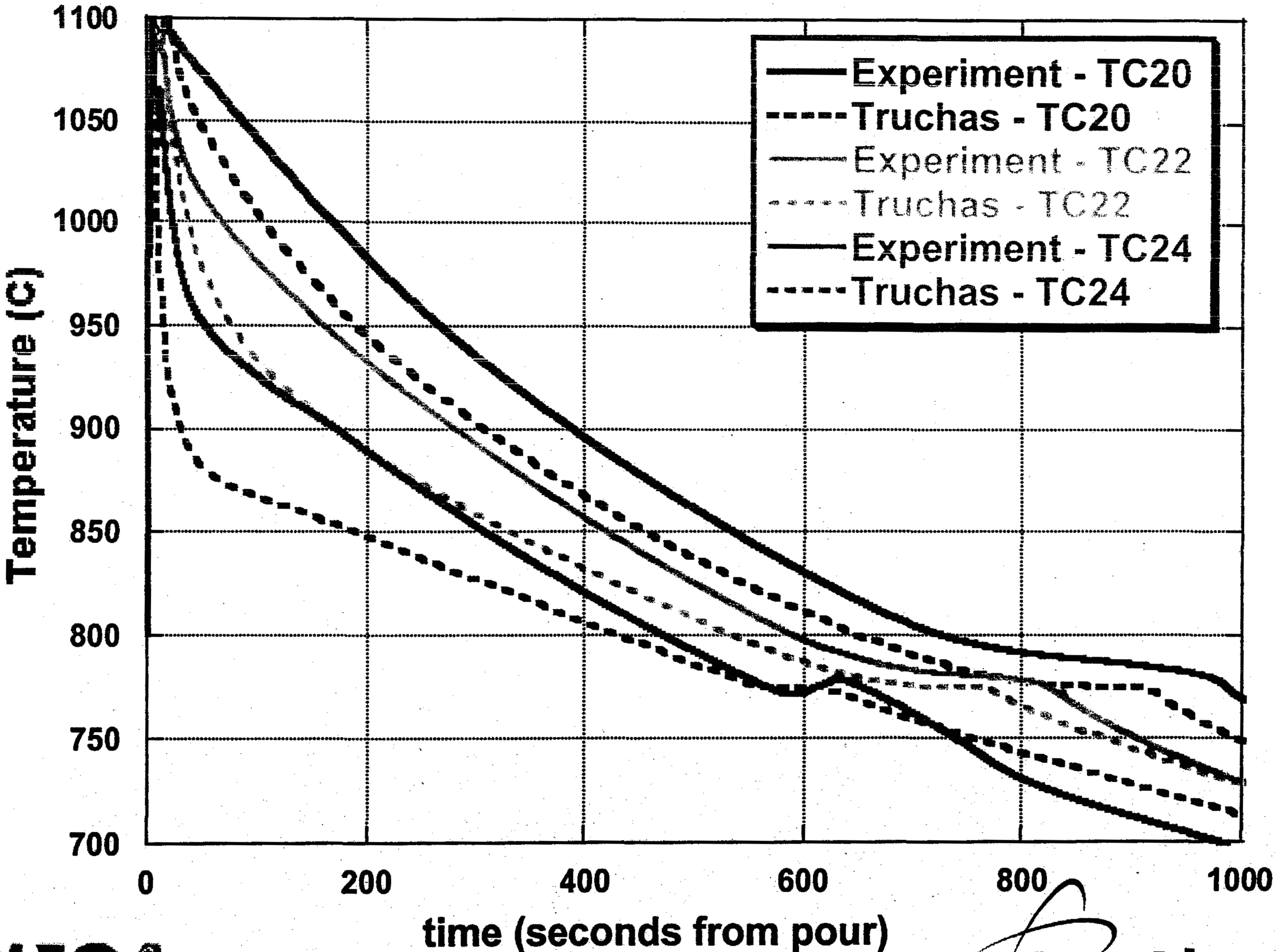
Temperature Through the Allotropic Phase Change



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Summary and Future Directions

•Computer simulation capabilities are continually increasing.

•Computer simulations can highlight the controlling processes in manufacturing.

•Continue development and testing for
electromagnetics and view factor radiation
thermomechanical model
grain growth model

•Gather more experimental information on material properties and boundary conditions

What is still needed Casting Simulations

Many codes can model fluid flow and heat transfer but to accurately simulate many castings more physics is needed.

- Initial mold temperatures and boundary conditions – only outer edge of mold couples with the induction field, the much of the mold stack is heated by conduction and radiation
  - Electromagnetic model
  - Radiation model with view factors
- Time/stress/position dependent heat transfer coefficient
- Stresses can develop within the casting to cause breakage of the mold and/or hot tearing of the metal
  - Thermomechanical model
- Microstructure/Alloy solidification–
  - Macrosegregation model
  - Dentritic growth and microsegregation model